XINXIN LIU (SHUNSUM LAU)

Master's Student in Physical Chemistry

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EDUCATION

MSc in Physical Chemistry

MOE Key Laboratory of Theoretical Chemistry of Environment; School of Environment, South China Normal University

2022 – 2025 | Guangzhou, China

CGPA: 3.99/5.00

BSc in Applied Chemistry

College of Materials and Energy, South China Agricultural University

2018 – 2022 | Guangzhou, China

CGPA: 3.93/5.00

DISSERTATION WORK

MSc Thesis

Analytical Electromagnetic Response Theory of HF/KS Energy: A Unified Treatment from Nonrelativistic to Relativistic Frameworks

- Constructed an analytical electromagnetic response theory based on quasi-energy derivatives within both HF and KS-DFT frameworks to avoid theoretical inconsistencies especially in dealing with dynamic electromagnetic response; response properties derived from the new theory are both comprehensive and gauge-independent
- Revealed that the widely adopted GIAO method in calculating magnetic response properties has little physical significance, and cannot fundamentally eliminate the gauge dependence in time-varying fields
- Extended the new approach to relativistic two- and four-component frameworks and incorporated the case of non-collinear exchange-correlation functionals
- Developed a Python code for implementing the above methods in PySCF

BSc Thesis

DFT Analysis of the Conversion Mechanism from Dihydroartemisinic Acid to Artemisinin

- Proposed a plausible reaction path
- Identified the initial dominant conformations of the reactant using xTB
- Computed the thermodynamic data using Gaussian
- Determined the rate-determining step of the reaction to optimize conditions for the drug production

CERTIFICATES

- CET-6 Certificate
- NCRE-2 Certificate
- the **Second Price Award** in the Preliminary Round of the 2019 "FLTRP·ETIC Cup" English Writing Contest

HOBBIES

Exploring Nature and the World
Observing the nature of things

Music Enthusiast
Enjoying quality music across various genres

Reading and Lifelong Learning
Pursuing continuous learning and meaningful discussions

LOOKING FOR

"To work in a progressive and dynamic research organization where one could solve scientific enigmas and contribute towards welfare of society"

TECHNICAL STRENGTH

Fortran	●○○○○
C/C++	●○○○○
Python	●●●●○
Bash	●●○○○
Tex	●●●●○
Git	●●●○○
MS Office	●●●●○

MOST PROUD OF

Top Performer in Master's Program
Achieved top position in the Diploma of Physical Chemistry program; Demonstrated a strong passion for natural sciences and a commitment to excellence in research

Knowledge Evolution
Going next level everyday by perpetual learning of scientific and technical knowledge

STRENGTHS

Thermodynamics & Statistical Mechanics | Linear Algebra | Quantum Chemistry | Vector and Tensor Analysis | Calculus | Classical Electrodynamics | Special Relativity | Careful and Earnest | Hard-working | Flexible and Adaptable

LANGUAGES

Chinese (Mandarin)	●●●●●
Cantonese	●●●●○
English	●●●○○